First-Principles Study of Uranium and Oxygen Diffusion in Uranium Dioxide UO_2

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Uranium dioxide (UO_2) attracts much interest due to its technological value as the standard nuclear fuel for pressurized water reactors. In order to get some comprehension in the evolution of the fuel properties under irradiation, the study of point defects and fission products is central. In particular, obtaining accurate formation and migration energies of point defects is essential in order to model the evolution of the microstructure of the material. First-principles electronic structure calculations can give direct insight into elementary transport processes at the atomic scale and the results can be used as input data in a multi-scale modeling scheme of the material properties, with direct links to modeling techniques such as classical molecular dynamics, kinetic Monte Carlo, ….

We will present here a first-principles study of uranium and oxygen diffusion in uranium dioxide. The activation energies obtained will be compared to recent experimental results [1, 2] for oxygen diffusion in UO_2.

Within standard Density Functional Theory (DFT), the strong correlations between the *5f* electrons of uranium in UO_2 are significantly underestimated and it still remains a challenge to accurately describe the electronic structure of UO_2. We will show that the addition of a Hubbard-like term in the so-called DFT+U [3] formalism improves the treatment of these electrons and succeeds in describing several bulk properties of UO_2, as well as the behaviour of its point defects [4,5].

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